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http://www.cas.org/ONLINE/UG/regprops.html

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chain nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-2 1-10 2-3 3-4 4-5 4-6 6-7 7-8 8-9

exact/norm bonds :

1-2 1-10 2-3 4-5 4-6 6-7 8-9

exact bonds :

3-4 7-8

G1:Cb,Cy,Hy

Match level:

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS

L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1

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G1 Cb, Cy, Hy

Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 15:42:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4156 TO ITERATE

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Karen Cheng

SEARCH TIME: 00.00.01

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COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 172.10 172.31

FULL ESTIMATED COST

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L3

5 L2

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OTHER SOURCE(S):

L3 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2004:220304 CAPLUS DOCUMENT NUMBER: 140:270877
TITLE: Preparation of the company of the

Preparation of heterocyclic-substituted amides as

Preparation of heterocyclic-substituted amides at cathepsin cysteine protease inhibitors
Boyd, Michaels Gagnon, Maccs Lau, Cheuks Mellon, Christopher Scheigetz, John
Merck Prosst Canada & Co., Can.
PCT Int. Appl., 118 pp.
CODEN: PIXXD2
Patent INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: English LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2004022526 A1 20040318 W0 2003-CA1346 20030903
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, II, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LL, LT, LU, LV, MA, MD, MG, MK, NN, MW, MX, MZ, NI, NO, NZ, CM, PG, PH, PL, PT, RO, RM, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SI, SZ, TZ, UG, ZW, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, TA, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, UM, MC, NL, PT, RO, SE, SI, SK, TS, ST, ST, TS, TR, BF, BJ, CF, CG, CI, CM, GA, GM, GQ, GW, ML, MR, NE, SN, TD, TG
CA 2495939 A1 20040318 CA 2003-266052 20030903
AU 2002266052 A1 20040318 CA 2003-2695039 20030903
AU 2002266052 A1 20050508 EP 2003-793540 20030903
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FR, RO, KC, VA, LT, RB, CZ, EE, HU, SK
US 2005137326 T 20051208 JP 2004-5313125 20030903
CTHER SOURCE(S): MARPAT 140:270877

MARPAT 140:270877

L3 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Absolute stereochemistry.

672328-15-3 CAPLUS Pentanamide, 2-[(R)-(4-bromophenyl)[4-(methylsulfonyl)phenyl]methoxy]-N-(cyanomethyl)-4-methyl-, (25)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

672328-19-7 CAPLUS
Pentanamide, 2-[(R)-(4-bromophenyl) (4-chlorophenyl)methoxy]-N-(cyanomethyl)-4-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute Stereochemistry.

Absolute stereochemistry.

Karen Cheng

ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

$$R^{9} \underbrace{\begin{array}{c} R^{8} & R^{7} & R^{4} \\ CD \end{array}_{n}^{R} X \underbrace{\begin{array}{c} R^{3} & H \\ O & R^{2} & R^{1} \end{array}}_{N} CN$$

Title compds. I [R]-4 = H, alkyl, alkenyl,etc.; X = O, S, 502, alkyl; R7-8 = H, alk(en/yn)lyl, haloalkyl, alkoxy, NO2, CN, etc.; D = (hetero)aryl, cycloalkyl, etc.; R9 = H, OH, CN, alkyl, etc.; n = 0-3] are prepared For instance, (55)-2-(4-bromophenyl)-5-isobutyl-1, 3-dioxolan-4-one (preparation given) is reacted with PhMgBr (Et2O, 2nCl2, -40°) and the resulting carboxylic acid coupled to aminoacetonitrile (DMF, HATU, Et3N) to give II. I are cysteine protease inhibitors, including but not limited to, inhibitors of cathepsins K, L, S and B and are useful for treating diseases in which inhibition of bone resorption is indicated, such as osteoprosis. They have the following structure: Formula (I). 672328-02-84 672328-15-39 672328-19-79
672328-22-2P 672328-25-5P, (25)-2-[(IR)-1-(4-Bromophenyl)-2-(4-chiorophenyl)-ehyl)oxyl-N-(cyanomethyl)-4-methyl-entanamide 672328-52-8P, N-(Cyanomethyl)-4-methyl-2-(phenyl(4-(piperazin-1-ylcarbonyl)phenyl)methoxylpentanamide 672328-55-3P, C(4-Bromophenyl)(1,3-5)
672328-57-19 672328-63-1P, 2-[(4-Bromophenyl)(1,3-5)
672328-97-97 672328-93-PP 672328-94-8P
672328-97-97 672328-91-3P 672328-94-8P
672328-97-97 672329-00-9P 672329-02-1P
672329-07-6P 672329-00-9P 672329-02-1P
672329-07-6P 67239-08-PP 672329-02-1P
672329-07-6P 67239-08-PP 672329-03-14-5P 674784-52-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); RAT (Reactant or reagent); USES (Uses)
(preparation of heterocyclic-substituted amides as cathepsin cysteine protease inhibitors)
672328-09-4 (APLUS
Pentanamide, 2-[(R)-(4-bromophenyl)phenylmethoxy]-N-(cyanomethyl)-4-methylPentanamide, 2-[(R)-(4-bromophenyl)phenylmethoxy]-N-(cyanomethyl)-4-methylPentanamide, 2-[(R)-(4-bromophenyl)phenylmethoxy]-N-(cyanomethyl)-4-methylPentanamide, 2-[(R)-(4-bromophenyl)phenylmethoxy]-N-(cyanomethyl)-4-methyl-

ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

672328-25-5 CAPLUS
Pentanamide, 2-{(1R)-1-{4-bromophenyl}-2-{4-chlorophenyl}ethoxy}-N-(cyanomethyl)-4-methyl-, (2S)- (9CI) (CA INDEX NAME)

672328-52-8 CAPLUS
Pentanamide, N-(cyanomethyl)-4-methyl-2-[phenyl[4-(1-piperazinylcarbonyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)

672328-55-1 CAPLUS Pentanamide, 2-[(3)-(4-bromophenyl)-2-thienylmethoxy]-N-(cyanomethyl)-4-methyl-, (25)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

143:97209
Synthesis of epothilones for use in pharmaceutical compositions as antitumor agents
Danishefsky, Samuel J.: Rivkin, Alexey; Yoshimura, Fumihiko; Chou, Ting-Chao; Gabarda, Ana E.: Dong, Huajin; Wu, Kaida; Moore, Malcolm A. S.; Dorn, David USA INVENTOR (S):

PATENT ASSIGNEE(S): U.S. Pat. Appl. Publ., 274 pp., Cont.-in-part of U.S. Ser. No. 435,408.
CODEN: USXXCO

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:						ent	USXX	co													
PF	PATENT NO.						DATE														
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US	2005	1434	29		A1		2005	0630		US 2	004-	9211	09		- 2	20040	818				
US	2004	0539	95		Al		2004	0318		US 2	003-	4020	04 .		2	20030	32B				
US	6921	769			B2		2005	0726							_						
US	2004	0539	10		Al		2004	0318		ŲS 2	003-	4354	08		- 3	0030	509				
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WC	2005	0842	22		A2		2005	0915		WO 2	005~	U\$60	51		20050228						
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										US 2	002-	4085	89P		P a	20020	906				
										US 2	002-	4231	29P		P :	20021	101				
										US 2	003-	4561	59P		P :	20030	320				
										US 2	003-	4020	04		A2 :	20030	328				
									٠	US 2	003-	4354	80		A2 :	20030	509				
										US 2	003-	4967	41P		P :	20030	821				

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(claimed compd.; synthesis of epothilone derivs. for use in
pharmaceutical compns. as antitumor agents)

RN 856240-85-2 CAPLUS
CN 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione,
10.14-dihydroxy-11,11,13,15tetramethyl-6-[(IE)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-3(trifluoromethyl)-, (1R,3E,6S,10S,13R,14S,15S,16S)- [9CI) (CA INDEX
NAME)

RN 856240-86-3 CAPLUS
CN 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione,
10,14-dihydroxy-11,11,13,15tetramethy1-6-[(1E)-1-methy1-2-(2-methy1-4-thiazoly1)etheny1]-3(trifluoromethy1)-, (1s,3E,6S,10S,13R,14S,15S,16R)- (9CI) (CA INDEX

856240-87-4 CAPLUS
7-Oxabicyclo(14.1.0)heptadec-3-ene-8,12-dione, 10,14-dihydroxy-3,11,11,13,15-pentamethyl-6-{(1E)-1-methyl-2-{2-methyl-4-thiazolyl}ethenyl}-, (1R,3Z,6S,10S,13R,14S,15S,16S)- (9CI) (CA INDEX NAME) RN CN

Karen Cheng

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) US 2004-548402P P 20 P 20040227

> US 2004-921109 A 20040818

> WO 2005-US6051 W 20050228

OTHER SOURCE(S): MARPAT 143:97209

Epothilone analogs, such as I [-A-B-, -C-D- = -C.tplbond.C-, -CH(R)-H(R)-H(R)-, -C(R):C(R])-; R, RI = H, alkyl, halogen, alkoxy, acyl, etc.; -A-B- = fused oxirane ring; -C-D- = fused cyclopropane or fused aziridine ring; R2 = aryl, heteroaryl, arylalkyl, heteroarylalkyl] are prepared as antitumor agents. The present invention also provides methods of treating cancer comprising administering a compound of

methods of treating cancer comprising administering a compound of ula I.

Thus, II was prepared via an intramol. methathesis macrocyclization synthetic sequence and showed good cell growth inhibition against various drug-resistant tumors.

856240-85-2P 856240-86-3P 856240-87-4P

856240-89-6P 856240-91-0P 856240-92-1P

856240-93-2P 856240-99-10P 856240-92-1P

856240-99-8P 856241-00-4P 856240-98-PP

856240-99-8P 856241-00-4P 856241-01-5P

856241-05-6P 856241-03-7P 856241-04-8P

856241-05-9P 856241-10-6P 856241-01-1P

856431-50-6P 856433-52-6P 856433-58-PP

856433-50-6P 856433-57-1P 856433-58-PP

856433-50-6P 856433-60-6P 856433-61-7P

856433-62-8P 856433-60-6P 856433-61-7P

856433-62-8P 856433-60-1P 856433-61-7P

856433-62-8P 856433-63-1P 856433-61-7P RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

856240-89-6 CAPLUS
7-0xablcyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-3,11,11,13,15-pentamethyl-6-{(1E)-1-methyl-2-{2-methyl-4-thiazolyl}ethenyl]-, (18,32,68,108,138,148,158,168)- (9CI) (CA INDEX

856240-91-0 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-

12,12,14,16-tetramethyl-7-{{1E}}-l-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-3-(trifluoromethyl)-, (1R,3R,5S,7S,1lS,14R,15S,16S,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856240-92-1 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-

12,12,14,16-tetramethyl-7-[{1E}-1-methyl-2-{2-methyl-4-thiazolyl}ethenyl}, 3-(trifluoromethyl)-, (1s,3R,5s,7s,11s,14R,15s,16s,17R)- {9CI} (CA INDEX

Absolute stereochemistry.
Double bond geometry as shown.

856240-93-2 CAPLUS
4,8-Dioxatricyclo(15.1.0.03,5)octadecane-9,13-dione, 11,15-dihydroxy3,12,12,14,16-pentamethyl-7-{(1E)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl}-, (1R,3R,5S,7S,11S,14R,15S,16S,173)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856240-96-5 CAPLUS 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-6-[(1E)-2-

[2-(hydroxymethyl)-4-thiazolyl]-1-methylethenyl]-11,11,13,15-tetramethyl-3-(trifluoromethyl)-, (18,3E,6S,10S,13R,14S,15S,16R)- (9CI) (CA INDEX NAME)

856240-97-6 CAPLUS
4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-7(1E)-2-[2-(hydroxymethyl)-4-thiazolyl]-1-methylethenyl]-12,12,14,16tetramethyl-3-(trifluoromethyl)-, (1R,3R,5s,7s,11s,14R,15s,16s,17s)-

(CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856240-94-3 CAPLUS
4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy3,12,12,14,16-pentamethy1-7-[(1E)-1-methy1-2-(2-methy1-4thiazoly1)etheny1]-, (1S,3R,5S,7S,11S,14R,15S,16S,17R)- (9CI) (CA INDEX

Absolute stereochemistry. Double bond geometry as shown.

856240-95-4 CAPLUS 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-6-{(1E)-2-

[2-(hydroxymethyl)-4-thiazolyl]-1-methylethenyl]-11,11,13,15-tetramethyl-3-(trifluoromethyl)-, (1R,3E,6S,10S,13R,14S,15S,16S)- (9CI) (CA INDEX NAME)

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856240-98-7 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-7-[(1E)-2-[2-(hydroxymethyl)-4-thiazolyl]-1-methylethenyl]-12,12,14,16-tetramethyl-3-(trifluoromethyl)-, (1S,2R,5S,7S,11S,14R,15S,16S,17R)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

856240-99-8 CAPLUS
7-0xabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-3,11,11,3,15-pentamethyl-6-[(1E)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-, (3Z,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856241-00-4 CAPLUS 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-

3,11,11,13,15-pentamethyl-6-{(1E)-1-methyl-2-(2-methyl-4-oxazolyl)ethenyl}-, (32,65,108,138,145,155)- (9CI) [CA INDEX NAME]

856241-01-5 CAPLUS 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-6-{(1E)-2-

[2-(hydroxymethy1)-4-thiazoly1]-1-methyletheny1]-3,11,11,13,15-pentamethyl-, (3Z,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856241-04-8 CAPLUS 7-0xabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-3,11,11,13,15-pentamethyl-6-[(1E)-1-methyl-2-(2-methyl-5-benzoxazolyl)ethenyl]-, (3Z,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

RN 856241-05-9 CAPLUS
CN 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione,
10,14-dihydroxy-11,11,13,15tetramethyl-6-[(18]-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-3(trifluoromethyl)-, (3E,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

RN 856241-06-0 CAPLUS

Karen Cheng

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856241-02-6 CAPLUS 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-6-[(1E)-2-

[2-(hydroxymethyl)-4-oxazolyl]-1-methylethenyl]-3,11,11,13,15-pentamethyl-, (3z,6s,10s,13x,14s,15s)- (9CI) (CA INDEX NAME)

856241-03-7 CAPLUS 7-0xabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-3,11,11,13,15-pentamethyl-6-{(1E)-1-methyl-2-(2-methyl-5-benzothiazolyl)ethenyl}-, (3Z,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

L9 ANSMER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione,
10,14-dihydroxy-11,11,13,15tetramethyl-6-{(1E)-1-methyl-2-(2-methyl-4-oxazolyl)ethenyl}-3(trifluoromethyl}-, (3E,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

RN 856241-07-1 CAPLUS
CN 7-0xabicyclo[14.1.0]heptadec-3-ene-8,12-dione,
6-[(1E)-2-[2-(aminomethyl)4-thiazolyl)-1-methylethenyl]-10,14-dihydroxy-3,11,11,13,15-pentamethyl-,
(3Z,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

RN 856241-08-2 CAPLUS CN 7-0xabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 6-[(1E)-2-[2-(aminomethyl)-4-oxazolyl)-1-methylethenyl]-10,14-dihydroxy-3,11,11,13,15-pentamethyl-, {32,65,103,13R,14S,155}- (9CI) (CA INDEX NAME)

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856241-10-6 CAPLUS 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-6-[(1E)-2-

[2-(hydroxymethyl)-4-thiazolyl]-1-methylethenyl]-11,11,13,15-tetramethyl-3-(trifluoromethyl)-, (3E,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

J

856241-11-7 CAPLUS 7-Oxabicyclo[14.1.0]heptadec-3-ene-8,12-dione, 10,14-dihydroxy-6-{(1E)-2-

[2-(hydroxymethy1)-4-oxazoly1]-1-methyletheny1]-11,11,13,15-tetramethyl-3-(trifluoromethy1)-, (3E,6S,10S,13R,14S,15S)- (9CI) (CA INDEX NAME)

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

856453-54-8 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-7-[(1E)-2-[2-(hydroxymethyl)-4-thiazolyl]-1-methylethenyl]-3,12,12,14,16-pentamethyl-, (78,118,14R,158,168)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

856453-56-0 CAPLUS
4,8-Dioxatricyclo[15.1.0.03,5]octadecone-9,13-dione, 11,15-dihydroxy-7[(1E)-2-[2-(hydroxymethyl)-4-oxazolyl]-1-methylethenyl]-3,12,12,14,16pentamethyl-, (73,118,14R,155,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856453-50-4 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-3,12,12,14,16-pentamethyl-7-{(1E)-1-methyl-2-{2-methyl-4-thiazolyl}ethenyl]-, (75,115,14R,15S,16S)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

856453-52-6 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-

3,12,12,14,16-pentamethyl-7-{(1E)-l-methyl-2-(2-methyl-4-oxazolyl)ethenyl}-, (7S,11S,14R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856453-57-1 CAPLUS
4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-3,12,12,14,16-pentamethyl-7-[(1E)-1-methyl-2-(2-methyl-5-benzothiazolyl)ethenyl]-, (7S,11S,14R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

856453-58-2 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-3,12,12,14,16-pentamethyl-7-{(1E)-1-methyl-2-(2-methyl-5-benzoxazolyl)ethenyl}-, (7S,11S,14R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856453-59-3 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-

12,12,14,16-tetramethy1-7-[(1E)-1-methy1-2-(2-methy1-4-thiazoly1)etheny1]-3-(trifluoromethy1)-, (7S,11S,14R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

856453-60-6 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-

12,12,14,16-tetramethyl-7-[(1E)-1-methyl-2-(2-methyl-4-oxazolyl)ethenyl]-3-(trifluoromethyl)-, (7s,11s,14k,15s,16s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856453-65-1 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-7-[(1E)-2-[2-(hydroxymethyl)-4-thiazolyl]-1-methylethenyl]-12,12,14,16-tetramethyl-3-(trifiuoromethyl)-, (75,115,14R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

856453-67-3 CAPLUS 4,9-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 11,15-dihydroxy-7-[(1E)-2-[2-(hydroxymethyl)-4-oxazolyl]-1-methylethenyl]-12,12,14,16-tetramethyl-3-(trifluoromethyl)-, (75,115,14R,15S,16S)- (9CI) (CA INDEX

Absolute stereochemistry.
Double bond geometry as shown.

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

856453-61-7 CAPLUS 4,8-Dioxatricyclo[15.1.0.03,5]octadecane-9,13-dione, 7-[(1E)-2-[2-

(aminomethyl)-4-thiazolyl}-1-methylethenyl}-11,15-dihydroxy-3,12,12,14,16-pentamethyl-, (7s,11s,14R,15s,16s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

856453-62-8 CAPLUS

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN
ACCESSION NUMBER: 2002:964345 CAPLUS
DOCUMENT NUMBER: 138:24952.
TITLE: Preparation of novel amino nitriles useful as reversible inhibitors of cysteine proteases
Hickey, Eugene R., 18 Bekkali, Younnes; Patel, Usha R.; Spero, Denice M.; Thomson, David S.; Young, Erick R. R. Boehringer Ingelheim Pharmaceuticals, Inc., USA PCT Int. Appl., 223 pp. CODEN: PIXXD2 PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English 1 PATENT NO. KIND DATE APPLICATION NO. DATE

OTHER SOURCE(S): MARPAT 138:24952

ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) chlorophenyl)methoxy]-1-cyanoethyl]amino]carbonyl]-3-methylbutyl ester (9C1) (CA INDEX NAME)

CH2-

478280-12-5 CAPLUS 2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-, 1-[[[1-cyano-2-[(4-methoxyphenyl)methoxy]ethyl]amino]carbonyl]-3-methylbutyl ester (9CI) (CA INDEX NAME)

478280-13-6 CAPLUS 2(1H)-130quinolinecarboxylic acid, 3,4-dihydro-, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl ester (9CI) (CA INDEX NAME)

Chralken or subst. ин- сн- сн2- о- сн2-

478280-22-7 CAPLUS
1-Piperazinecarboxylic acid, 4-phenyl-, 2-[(1-cyano-1-methylethyl)amino]-2-oxo-1-phenylethyl ester (9CI) (CA INDEX NAME)

478280-23-8 CAPLUS 5-14-pyridinyll . 2-111 cyano 3(Uses)
(prepn. of novel amino nitriles as reversible inhibitors of cysteine proteases)
478279-49-1 CAPLUS
4-Morpholinecarboxylic acid, (1S)-1-[[[(1R)-1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

478279-54-8 CAPLUS
4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl ester (9CI) (CA INDEX NAME)

ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

478280-24-9 CAPLUS
1-Piperidinecarboxylic acid, 4-[[4-[[1-[[(1-cyano-2-phenylethy)] amino]carbonyl]propoxy]carbonyl]-2-thiazolyl]amino]-, ethylester (9CI) (CA INDEX NAME)

478280-30-7 CAPLUS
4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-(cyclopropylmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

CH2-Ph

478280-34-1 CAPLUS
2-Naphthalenecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl ester (9CI) (CA INDEX NAME)

. СН— СН2**— О—** СН2— Р h

(phenylmethoxy) sthyl]amino]-1-(cyclopropylmethyl)-2-oxosthyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

478280-37-4 CAPLUS
2-Naphthalenecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-(cyclopropylmethyl)-2-oxpethyl ester (9Cl) (CA INDEX NAME)

478280-52-3 CAPLUS
Benzo[b]thiophene-2-carboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino[carbonyl]-3-methylbutyl ester (9CI) (CA INDEX NAME)

478280-53-4 CAPLUS
2-Benzofurancarboxylic acid, 5-[2-(4-morpholinyl)ethoxy]-,
1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl ester
(SCI) (CA INDEX NAME)

ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

478280-58-9 CAPLUS
2(1H)-Infoquinolinecarboxylic acid, 3,4-dihydro-, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl)-3,3,3-trifluoropropyl ester (9CI)
(CA INDEX NAME)

478281-00-4 CAPLUS
4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-4,4-dimethylpentylester (9CI) (CA INDEX NAME)

478281-03-7 CAPLUS
4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-4-methylpentyl ester (9CI) (CA INDEX NAME)

RN 478281-06-0 CAPLUS
CN 4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]car

Karen Cheng

ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
2-Benzofurancarboxylic acid, 1-4[[1-cyano-2-(phenylmethoxy)ethyl]amino]car
bonyl]-3-methylbutyl ester [961) (CA INDEX NAME)

478280-55-6 CAPLUS
2-Benzofurancarboxylic acid, 3-methyl-, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl ester (9CI) (CA INDEX NAME)

478280-56-7 CAPLUS
2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-, 1-[[[2-[(3-carboxyphenyl)methoxy]-1-cyanoethyl]amino]carbonyl]-3-methylbutyl ester
(9CI) (CA INDEX NAME)

478280-57-8 CAPLUS
2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3,3-difluoropropyl ester (9CI) (CAINDEN NAME)

ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) bonyl]-3,3,4,4-tetramgefylpentyl ester (9CI) (CA INDEX NAME)

478281-09-3 CAPLUS
4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3,3-dimethylpgntyl ester (9CI) (CA INDEX NAME)

478281-12-8 CAPLUS 4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-{phenylmethoxy}ethyl]amino]carbonyl]-3,3,4-tptmethylpentyl ester (9CI) (CA INDEX NAME)

478281-15-1 CAPLUS
4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-cyclohexyl-3-methylbutyl ester (9CI) (CA INDEX NAME)

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L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continu

RN 478281-18-4 CAPLUS
CN 4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-cyclohexylpropyl ester (9CI) (CA INDEX NAME)

RN 478281-21-9 CAPLUS
CN 4-Morpholing Carboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carboxyl-3-pyenylpropyl ester (9CI) (CA INDEX NAME)

RN 478281-25-3 CAPLUS
CN 4-Horpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1(cyclohexylmethyl)-2-oxoethyl ester (SCI) (CA INDEX NAME)

RN 478261-28-6 'CAPLUS
CN 4-Horpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-2oxo-1-(phenylmethyl)ethyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
[(3,4-dichlorophenyl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

RN 478281-43-5 CAPLUS
CN 4-Morpholinecarbowylic 3-1d, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-cyclohexyl-2-oxoethyl_aster (9CI) (CA INDEX NAME)

RN 478281-46-8 CAPLUS
CN 4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1(2-naphthalenylmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

RN 478281-49-1/CAPLUS
CN 4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1[(decahydro-2-naphthalenyl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

[(4,4-dimethylcyclohexyl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

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L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

O CH2-Ph

C-O-CH-C-NH-CH2-O-CH2-Ph

O CN

RN 4782(1-31-1 CAPLUS CN 4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-[(1-methylcyclohexyl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

RN 478281-34-4 CAPLUS
CN 4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carboxyl]-3,3-dimethylbutylester (9CI) (CA INDEX NAME)

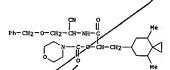
RN 478281-37-7 CAPLUS
CN 4-Morpholinecarboxylic acid. 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methyl-3-buteny/ester (9CI) (CA INDEX NAME)

RN 478281-40-2 CAPLUS CN 4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Me CN CN CN CNH-CH-CH-CH₂-O-CH₂-Ph

RN 478281-\$5-9 CAPLUS
CN 4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1[(4,8-dimethyl=piro(2.5)cct-6-yl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)



RN 478281_58-2 CAPLUS
CN 4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1[(2,2-dimethylcyclohexyl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

RN 478281-61-7 CAPLUS
CN 4-Morpholinecarboxylic acid, 2-[{1-cyano-2-(phenylmethoxy)ethyl)amino]-2oxo-1-[(3,3,5,5-tetramethylcyclohexyl)methyl)ethyl ester (9CI) (CA INDEX
NAME)

CN 4-Morpholinecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1[(2,3-dihydro-1H-inden-1-yl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued

CH2-CH-O-C-N
0 | CN
| C-NH-CH-CH2-O-CH2-Ph

RN 478281-67-3 CAPLUS
CN 4-Morpholinecarboxylic acid, 2-[[1-cyano---(phenylmethoxy)ethyl]amino]-1[(2,3-dihydro-1H-inden-2-yl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

RN 478281-70-8 CAPLUS

A-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-(methylsulfonyl)gropyl ester (9CI) (CA INDEX NAME)

C-NH-CH-CH₂-O-CH₂-Ph

RN 478281-73-1 CMPLUS CN 4-Morpholinecytoxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-(1-naphthalen/lmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN C-NH-CH-CH2-O-CH2-Ph

RN 478281-85-5 CAPLUS
CN 4-Morpholinecarboxylic acid, [[[1-cyano-2-(phenylmethoxy)ethyl]amino]carboxyl-2-methylbutyl ester ASCI) (CA INDEX NAME)

O CN
O C-NH-CU-CH2-O-CH2-Ph
O C-O-CH-Off-Et
Me .

RN 478281-88-8 CAPLUS
CN 2(1H)-1soquinolinecarboxylic cid, 3,4-dihydro-, 2-[[1-cyano-2-(phenylmethoxy) ethyl] aminol 1-(2,2-dimethylcyclopropyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

CN NH-CH-CH₂-O-CH₂-Ph

RN 478281-89-9 CAPLUS
CN 2(IH)-Isoquinolinecarboxylic acid, 3,4-dihydro-, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-cyclopropyl-2-oxoethyl ester (9CI) (CA INDEX NAME)

NH-C-O-CH₂-Ph

(phenyimethoxy) ethyl] amino] -2-oxoethyl ester (9CI) (CA INDEX NAME)

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L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

C=0

CN

CN

CH2

CH2

RN 478281-76-4 CAPLUS
CN 4-Morpholinecarboxylic acid, 1-([1,1'biphenyl]-4-ylmethyl)-2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-2-oxoeylyl ester (9CI) (CA INDEX NAME)

Ph CH2-CH- CH2-Ph

RN 478281-79-7 CAPLUS
CN 4-Morpholimecarboxylic acid, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1[(4-methoxyphenyl)methyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

MeO CH CH-CH-CH-CH2-Ph

RN 478281-83-2 CAPLUS
CN 4-Morpholinecarboxylic acid, 1-[[[1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-(methylthio)propyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 478281-91-3 CAPLUS
CN 2(1H)-1soquinolinecarboxylic acid, 4-dihydro-, 2-[[1-cyano-2-(phenylmethoxy)ethyl]amino]-1-methyl-2-oxoethyl ester (9CI) (CA INDEX NAME)

0 CN C-0-0H-5 NH-CH-CH₂-0-CH₂-Ph

RN 478281-92-4 CAPLUS
CN 2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-, 1-[[(1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]propyl ester (9CI) (CA INDEX NAME)

C-O'-CH-Et C-NH-CH-CH₂-O-CH₂-Ph

RN 478281-93-5 CAPLUS
CN 2(1E)-Isoquinolinecarboxylic acid, 3,4-dihydro-, 1-{{[1-cyano-2-(phenylmethoxy)ethyl]amimp]carbonyl]butyl ester (9CI) (CA INDEX NAME)

O CH-Pr-n C-NH-CH-CH2-O-CH2-Ph

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

477938-71-9 CAPLUS
4-Morpholinecarboxylic acid, (1R)-2-[(cyanomethyl)amino]-1-[[[[2-(difluoromethoxy)phenyl]methyl]-2loxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

477938-85-5 CAPLUS
1-Pytrolidinecarboxylic acid, (15)-2-[(cyanomethyl)amino]-1-(cyclohexylmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

477938-86-6 CAPLUS 4-Morpholinecarboxylic acid, (1S)-2-[(cyanomethyl)amino]-1-(cyclohexylmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)

The invention relates to compds. R3C(X2)(X7)CO-X1 [X1 = NHC(R1)(R2)X3 or NHM4; X2 = H, F, OH, OAK, NHR15, or NR17R18; X7 = H or X2 = X7 = F, R3 = alkyl or CR62X6; X3 = cyano, CR7R8R16, CR6(OR6)2, CH2COR16, CH2CHSCOR5, COCP2CONR52, COCONR5R6, COCC2R5, COCH2OR5, COCH2NR6SO2R5, or COCOR5; where R5 is H or (un)substituted alkyl; R6 is H, OH or NR5R6 is a ring; R7 is H, alkyl; and R8 is OH or CR7R8 are oxo; R16 is H, X4, CF3, NR6OR6, etc.; X4 comprises a heteromono or -bicyclic ring; R1 = H, alkyl; R2 = H, cyano; R2 = H, cyano, -X5-NR122, -X5-NR12COR12, etc., where X5 is a bond or alkylene and R12 is H, alkyl; n chaloalkyl; or CR1R2 may form a ring; R4 = alkylene-NR122; alkylene-NR122, -X5-NR12COR12, etc.; X6 = -X5-NR122, -X5-NR12COR12, etc.; R15 = H, alkyl; R17, R18 = (un)substituted alkyl (with provisos)] and their pharmaceutically acceptable salts and N-oxides as selective cathepsin S inhibitors for use as therapeutic agents. Thus, ester I was prepared via amide coupling reaction and showed Xi .ltorsim. 0.01 µH for inhibition of cathepsin S. 717938-45-69 477938-94-69 477938-95-69 477938-96-68 477938-97-99 477938-94-69 47797938-95-97-97 477938-96-69 477938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 477938-94-69 47797938-97-99 47797938-94-69 47797938-97-99 4

(Uses) (preparation of amide compds. and compns. as selective cathepsin S inhibitors) 477938-42-4 CAPLUS (Cyclohexanperopanamide, N=(cyenomethyl)-a-(phenylmethoxy)- (9CI) (CA INDEX NAME) Ph-CH2-0 477938-46-8 CAPLUS

477938-46-8 CAPLUS

A-HOEPHOTINGUETBONFIE acid, (IR)-2-[(cyanomethyl) aminoj-2-oxo-[((phenylmethyl) sulfonyl)methyl)ethyl ester (9CI) (CA INDEX NAME) Absolute stereochemistry.

(Continued)

ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

1-Piperazinecarboxylic acid, 4-ethyl-, (15)-2-[(cyanomethyl)amino]-1-(cyclohexylmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

4
777938-88-8 CAPLUS
1-Pyrrolidinecarboxylic acid, 2-(hydroxymethyl)-, (15)-2[(cyanohethyl)amino]-1-(cyclohexylmethyl)-2-oxoethyl ester, (25)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

477938-92-4 CAPLUS 1-Azetidinecarboxylic acid, (1S)-2-((cyanomethyl)amino)-1-(cyclohexylmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)

477938-94-6 CAPLUS 1-Piperidinecarboxylic acid, (15)-2-[(cyanomethyl)amino]-1-(cyclohexylmethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

477938-96-8 CAPLUS
1-Pycrolidinecarboxylic acid, 3-hydroxy-, (15)-2-[(cyanomethyl)amino]-1-(cyclohexylmethyl)-2-oxoethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

477938-97-9 CAPLUS
1-Pyrrolidinecarboxylic acid, 3-hydroxy-, (1S)-2-[(cyanomethyl)amino]-1-(cyclohexylmethyl)-2-oxoethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
11711E:
INVENTOR(S):
PATENT ASSIGNEE(S):
PATENT ASSIGNEE(S):
COURTY PAT

FAMILY ACC. NUM. COUNT:

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											WO	2002-	·US65	33		2	0020	301
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								ZA,									,	
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OTHER		MINCE						127.	2220		wo	2002-	.0202	33		* 2	0020	301
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R SOURCE(S): MARPAT 137:232908
The invention relates to a novel class of compds. R5-(E) n-D-X-CR3RACOMECRIRZON (R1 = H, (halo) alkyl, or (halo) alkenyl or R1R2C is a cycloalkyl ring optionally substituted by alkyl, hydroxyalkyl, or halogen, R3, R4 = H, alkyl or alkenyl optionally substituted by cycloalkyl or halogen or R3R4C is cycloalkyl, cycloalkenyl or heterocyclyl optionally substituted by alkyl, halo, hydroxyalkyl, hydroxy, alkoxy, or keto; X = NH, NR6, NHSO2, O, CR7R80, CCR7R8, CR7R8-CR7R8-CS, SO2CR7R8, CR7R8, CR7R8-CR7R8-CS, SO2CR7R8, CR7R8, CR7R8-CR7R8-CR7R8-CS, SO2CR7R8-CR7R8, charge R6 = alkyl or R6 and R4 form a 4-12 membered heterocyclyl ring system which is optionally substituted and R7, R8 = H or alkyl; D, E = (un)substituted aryl, heteroaryl, cycloalkyl, or heterocyclyl n = 1-2; R5 = H, alkyl, alkenyl, alkoxy, halo, nitro, cyano, amino, aryl, heteroaryl, cycloalkyl, heteroaryl, cycloalkyl, sakenyl, alkoxy, halo, nitro, cyano, saino, aryl, heteroaryl, cycloalkyl, heteroaryl, cycloalkyl, charge cycloskyl, cozh, cycloalkyl, alkonyl, groups, etc.] and their chargestically-acceptable and the specific derivatives are cyclosed.

C4H9N2-p-C6H4-p-C6H4-L-Leu-NHCH2CN (C4H9N2 = 1-piperazinyi) was prepared from L-leucine, 1,4-dibromobenzene, aminoacetonitrile hydrochloride, and 4-[4-(tert-butoxycarbonyl)-1-piperazinyl]phenylboronic acid (preparation

Karen Cheng

ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued) 477938-98-0 CAPLUS
4-Morpholinecarboxylic acid, (15)-1-[[(cyanomethyl)amino]carbonyl]-3-cyclohexylpropyl ester (9CI) (CA INDEX NAME)

L3

ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) given). The product was used to prep. a pharmaceutical compn. 459160-52-2P 459162-53-9P 459162-77-7P 459162-78-8P 459162-79-9P 459162-82-4P 459162-83-5P RE: PAC (Pharmacological activity); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea)

(preparation of N-cyanomethyl amides as cathepsin cysteine protease inhibitors)
459160-52-2 CAPLUS
Fentanam.de, N-(cyanomethyl)-4-methyl-2-[[4'-(1-piperazinyl)][1,1'-biphenyl]-4-yl]methoxyl- (9CI) (CA INDEX NAME)

459162-53-9 CAPLUS Pentananido, 2-([1,1'-biphenyl]-4-ylmethoxy)-N-(cyanomethyl)-4-methyl-(SCI) (CA INDEX NAME)

459162-77-7 CAPLUS
1-Piperazinecarboxylic acid, 4-[3'-[[1-[[(cyanomethyl)amino]carbonyl]-3-methylbutoxy]mathyl][1,1'-biphenyl]-4-yl]-, 1,1-dimethylathyl ester (9CI) (CA INDEX NAME)

459162-78-8 CAPLUS

10525264

ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
1-Piperazinecacboxylic acid, 4-[4'-[{1-[[(cyanomethyl) amino]carbonyl]-3-methylbutoxy]methyl][1,1'-biphenyl]-4-yl]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

459162-79-9 CAPLUS 1-Piperazinecarboxylic acid, 4-[2'-[[1-[[(cyanomethyl)amino]carbonyl]-3-methylbutoxy]methyl][1,1'-biphenyl]-4-yl]-, 1,1-dimathylethyl ester (9CI) (CA INDEX NAME)

459162-82-4 CAPLUS
Pentanamide, N-(cyanomethyl)-4-methyl-2-[[4'-{1-piperazinyl}]{1,1'-biphenyl}-2-yl]methoxy]- (9CI) (CA INDEX NAME)

 $459162-83-5 \quad CAPLUS \\ Pentanamide, N-(cyanomethyl)-4-methyl-2-\{\{4'-\{1-piperazinyl\}\{1,1'-biphenyl\}-3-yl\}methoxy\}- (9CI) \quad (CA INDEX NAME)$

L3 ANSWER 5 OF 5
ACCESSION NUMBER:
1994:557664 CAPLUS
DOCUMENT NUMBER:
1171E:
121:157664
3-aryluracil derivatives and the use thereof for weed control
INVENTOR(5):
PATENT ASSIGNEE(S):
COURCE:
CODEN: PIXXD2
PATENT TYPE:
LANGUAGE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

COPPLIGHT 2007 ACS on STN
121:157664
CAPLUS
121:157664
3-aryluracil derivatives and the use thereof for weed control
COLDEN: PIXXD2
PATENT INTORNATION:

121:157664
3-aryluracil derivatives and the use thereof for weed control
Control
Countrol
Ciba-Geigy A.-G., Switz.
PCT Int. Appl., 54 pp.
CODEN: PIXXD2
Patent INFORMATION: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.						KIND DATE				APP	LIC		DATE							
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WO	9410	155			A1		1994	0511		WO	199	93-	EP28	02			19	931	012	
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BR	9305	683			Α		1996	1203		BR	199	93-	5683				19	931	012	
PRIORIT	Y APP	LN.	INFO	. :						СН	199	92-	3310							
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OTHER S	ouner.						101.	1576				,,,	Zu	UL		•	.,	331	012	
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The title 3-aryluracils I (W = aminocarbonyl group; R2 = halo, cyano, alkyl, etc.; R3 = H, F; R4 = H, halo, alkyl, etc.; R5 = alkyl, haloalkyl, etc.; R6-R9 = H, alkyl, etc.; R10, R11 = H, alkyl, alkenyl, etc.; m = 0-1)

Karen Cheng

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

$$\label{eq:chi2-optimize} \begin{array}{c} 0 \\ \text{C-NH-CH}_2\text{-CN} \\ \text{CH}_2\text{-O-CH-Bu-i} \end{array}$$

459164-65-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-cyanomethyl amides as cathepsin cysteine protease inhibitors)
459164-65-9 CAPLUS
Pentanamide, 2-[(4-bromophenyl)methoxy]-N-(cyanomethyl)-4-methyl- (9CI)
(CA INDEX NAME)

ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) were disclosed. An example compd., 1-methyl-3-(4-morpholinyl)-3-oxopropyl 2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1-pyrimidinyl]benzoate ([I] was prepd. Compds. I are suitable as active ingredients of herbicidal compns. for weed control. 157307-15-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)
157307-15-8 CAPLUS
Benzoic acid, 2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl)-, 2-[(cyanomethyl) amino]-1,1-dimethyl-2-oxoethyl ester (9CI) (CA INDEX NAME)